

# BioCoRE: A Biological Collaborative Research Environment

## Abstract

BioCoRE is a freely available web-based collaborative environment designed to enhance the biomedical research process and promote training. By using a standard web-browser (on a handheld PDA or desktop or laptop computer) scientists create projects and invite collaborators to join. All project data is secure and can be shared only by the specific project team. Researchers use BioCoRE to submit jobs to supercomputers or other remote sites, view molecules together across distances and easily create input files for supercomputer runs. BioCoRE features a synchronous and asynchronous chat, a project-wide "bookmarks" file that enables the sharing of weblinks as well as a web-based filesystem that is accessible to the BioCoRE project members. This filesystem is used to share files of interest and to simplify publication preparations via a seamless transport of document files among project members.

Summary pages within BioCoRE regularly inform the project team of the project status, including individual tasks of each team member. BioCoRE sessions are automatically recorded and can be reviewed later by the project leader and the other team members.

## Concept

The overarching goal driving BioCoRE development is to provide a secure environment that will enhance the research process by improving the collaboration between biomedical researchers located at either the same institution or at geographically distant places and by facilitating the transparent use of and communication between existing programs, tools, and databases. A built-in evaluation component in BioCoRE guarantees the ability to assess the usage and acceptance of the BioCoRE environment. Scientists within BioCoRE interact in both synchronous and asynchronous fashion with each other or with the modeling tools via a common infrastructure. BioCoRE efforts are geared towards meeting essential needs of cutting-edge biomedical research and for addressing lacking capabilities of existing software packages. To that end, BioCoRE is designed to provide the following functionality:

- resource allocation and remote job submission to access data storage and queuing systems;
- integrated interfaces to analysis tools for analyzing shared data, reviewing results, and for accessing genomic and structural databases;
- record keeping to save and retrace history of projects, log online sessions, search past records, make annotations to projects, and to record references to data used in or generated by BioCoRE projects;
- collaborative visualization to permit distant researchers to view and share control of a common molecular representation;
- unified data repositories, unrestricted by local disk space limitations, to facilitate visualization, analysis, remote simulations, and access to digital libraries;
- communication via chat rooms, news groups, white boards, etc. recorded for later reference or playback;
- audio/video capabilities for meetings, lectures, and presentations;
- report and publication tools to provide collaborators direct access to the joint text and figures in preparation;
- mentoring and training capabilities to equip the principal investigators with more systematic ways to guide research and advise students;
- creation of training modules will be supported;
- monitoring capabilities to follow the progress of other collaborators.

## Collaborative Projects

The screenshot shows the BioCoRE web interface. At the top, there are navigation buttons (Back, Forward, Reload, Home, Search, Netscape, Print, Security, Stop, Step). Below that, a 'PROJECTS' section lists 'ATPase' as the current project. A 'Summary: Project 'ATPase'' section provides project details. A 'Recent Message Board Entries' section lists recent activity. A 'Job Management status' table shows the status of various jobs.

Name	Account	Type	Status	Last updated
ATP_Synthase_2	otwada-short	NAMD	Complete	Tue Sep 18 11:44:15 CDT 2001
stphase-1	NCSA Origin	NAMD	Complete	Tue Sep 18 11:40:32 CDT 2001

A Website Link Library lets project members share interesting weblinks with their collaborators. Users add links to the Library, and other project members can follow the links and add links of their own. Links are organized by topic, and automatically sorted by popularity.

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## Collaborative Visualization

The screenshot shows the VMD (Visual Molecular Dynamics) software interface. It displays a 3D molecular structure of a protein, likely ATPase, with various atoms and bonds represented in different colors. The interface includes a menu bar (File, Edit, View, Go, Communicator), a toolbar, and a main display area. A 'VMD States' dialog box is open, showing a list of saved states and options to load or save states. A 'vmd console' window at the bottom shows system messages.

Via BioCoRE, members use VMD (Visual Molecular Dynamics; <http://www.ks.uiuc.edu/Research/vmd/>) and easily share molecular representations with their collaborators. Users can load their molecule files from BioCoRE's integrated filesystem and set up molecules in any state they deem insightful. Users can "save" the preferred state to the project they are working on in BioCoRE. Other collaborators in that project can then choose to view that state any time. By simply clicking on a link within BioCoRE, VMD is automatically started, the PDB file downloaded to one's computer, and the molecular representation modified to be in the exact same configuration as when the user saved it.

This functionality, coupled with the Control Panel chat, allows real-time discussion and display of molecules with one's collaborators. As everything in BioCoRE is automatically archived, one can always go back and view earlier saved states and communication from project members even if one were not logged into BioCoRE at the time the state was originally saved.

## Simulation Configuration "Wizard"

BioCoRE's Simulation Configuration "wizard" simplifies the generation of configuration files for NAMD (a parallel Molecular Dynamics code designed for simulation of large biomolecular systems; <http://www.ks.uiuc.edu/Research/namd/>). Due to the complexity of NAMD, setting up configuration files can be a challenge, especially for new users. BioCoRE has a graphical interface to aid in this process. Users "fill in the blanks" with applicable values for the simulation they wish to perform. The configuration options are divided according to category and users can see and edit the final version before saving.

The configuration wizard is intelligent enough to check for common input errors users make in configuration files (such as having illegal negative values) and will warn the user before saving. Thus, one does not have to wait until the job has been submitted to the supercomputer (possibly having sat in the queue for days) to discover errors. Users can load configuration files from their own computer or directly from BioCoRE's integrated filesystem.

The screenshot shows the BioCoRE Simulation Configuration Wizard interface. It is a web-based form with multiple sections for configuring simulation parameters. Sections include 'FORCE FIELD', 'ENSEMBLE', 'INITIAL', 'OUTPUT', 'PROTOCOL', and 'ADDITIONAL'. Each section contains various input fields, checkboxes, and buttons for selecting files or values. The interface is designed to be user-friendly and guide the user through the complex process of setting up a simulation.

## Acknowledgements

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## Supercomputer Job Management

BioCoRE offers web-based access to researchers' supercomputer accounts. Users "register" their supercomputer accounts (at NCSA, PSC, elsewhere) with BioCoRE, and BioCoRE can then submit and monitor supercomputer jobs on their behalf.

Once the user has registered their account, they simply tell BioCoRE that they want to run a job, such as a NAMD simulation. Upon giving information about configuration file names, number of processors needed, etc., BioCoRE will automatically create an appropriate queue submission script for the supercomputer they select.

Users can have multiple jobs running on multiple computers and BioCoRE allows the user to track them all from a single web page. BioCoRE can monitor the queue status and the user is able to see via the web when their jobs have started and finished. BioCoRE automatically deposits run information in the integrated filesystem.

BioCoRE allows job submissions via Globus to any supercomputer using the Alliance Globus certificate (which includes NCSA and SDSC).

The screenshot shows the BioCoRE web interface for job management. It displays a 'Jobs' section with a table of running jobs. The table includes columns for Name, Account, Project, Type, Status, and Last updated. A 'Select a job to Edit, Delete, or View Details' section is visible below the table.

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## Integrated, Shared Filesystem and Web-based Molecular Visualization

The screenshot shows the BioCoRE web interface for file management and molecular visualization. It displays a 'BioCoRE Control Panel' with a file browser showing a directory structure. A 'Netscape: BioFS file Properties: 1 ABV.pd' window is open, showing file information. A molecular structure is visible in the background.

BioCoRE features a built-in web-accessible filesystem that is available to all members. Each project shares a file space and project members can deposit files for collaborators to view and download. Additionally, each user can use a personal file space where they can deposit files not necessarily related to a particular research project they are involved in.

For PDB molecular data files, BioCoRE has a web-based Java 3D molecule viewer, JMV. With JMV (<http://www.ks.uiuc.edu/Development/jmv/>) one can rotate molecules, change representations and coloring, all from a web page. This is very convenient for instances when one might be at a conference or elsewhere with no access to an installed program like VMD.

## BioCoRE Server Software Available For Download

Researchers are encouraged to use the freely available BioCoRE collaborative server developed by the Theoretical Biophysics group (<http://www.ks.uiuc.edu/Research/biocore/>), an NIH Resource for Macromolecular Modeling and Bioinformatics. This server is regularly updated and can be used for either general or discipline-specific collaborative work.

The BioCoRE collaborative server software is freely available for installation, providing local users with greater speed and security in accessing BioCoRE. For easy installation, the server software has been written using standard open-source packages.